DFTB study of the electronic and magnetic properties of titanium carbide Mxene

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Two-dimensional (2D) materials metal carbide MXenes ($Ti_{n+1}C_n$; n=1, 2, 3, 4) has attracted a lot of attention recently [1, 2], due to its promising physical and chemical properties [3, 4]. It was shown that after the synthesis process, the MXenes are usually functionalized with O and F atoms, or -OH group [5, 6]. Moreover, the electronic, optical and magnetic properties of MXenes are affected by the surface termination [5-7].

Our computational study of the electronic and magnetic properties of MXenes have been performed using a calculation method that combines density functional theory (DFT) based ground state calculation with tight binding approach. The Self Consistent Charge Density Functional Tight Binding method (SCC-DFTB) which is an approximate, parametrised form of DFT [8] gives a response of the need for approximate methods. DFTB is is capable of targeting the studied MXene systems. This method allows us to optimize the "computational costs" with reasonable accuracy for large MXene systems. Here, we show good performance of DFTB approach to investigate the electronic and magnetic properties O-functionnalazed Titanium carbide MXene.

DFTB calculations provide a reasonable electronic structure and magnetic properties of the studies MXenes. We consider mainly Ti_2C which have magnetically ordered ground states. The magnetization is attributed, mainly, to the 3d electrons of surface Ti atoms. However, when two surfaces of Ti_2C monolayer are saturated by O atoms, the magnetism is spontaneously removed and Ti_2CO_2 shows a semiconducting behaviour.

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